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A COMPUTERIZED SYSTEM FOR DATA HANDLING

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ABSTRACT

An open-ended "menu"-directed, set of FORTRAN programs are being written to produce graphic displays and otherwise process data from a number of different surface science instruments. To date, programs have been written for x-ray photoelectron (XPS, ESCA) and Auger spectroscopies. The data produced by these instruments are stored in a Nicolet, Model 1074, hard-wired, multichannel, data analyzer in 1024 channels. These 1024 data points are sent serially to the computer. The operator then enters the sample information and experimental parameters of the spectrum. The spectra can then be manipulated using a variety of interactive graphic routines.

The basic hardware for the system consists of an LSI-11/2, 10 Mbyte disk drive and a 4027 Tektronix color graphics terminal.

These programs have been designed with the aid of top-down structure diagrams. These diagrams will be used to discuss the general feature of the programs and how they interact. Software, hardware, future expansion and user reaction will also be discussed.

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This paper describes the computer automation of several surface science techniques. The project is only partially complete, and will continue to improve and expand. The aim of this automation project is to provide an easily used, expandable, interaction system utilizing computer graphics to rapidly acquire, store, recall, and process data from different surface science techniques. To date, the ESCA/UPS technique and the AUGER technique have been implemented.

The computer hardware chosen for this task is shown in Figure 1. By utilizing a Tektronix 4027 color graphics terminal, two identical systems could be purchased for less than $40K of capital equipment money. The LSI-11/2 computer was chosen because of the extensive software available and the ability to upgrade to the more powerful 11/23 processor.

The software for the automation is being developed in-house in FORTRAN-IV. The design goal is to produce a system that is simple to learn, even by the casual user, and that is easily extended to include additional techniques. To accomplish this goal, the system uses menus whenever the operator must make a choice from two or more options. Whenever numerical input is required, the user is prompted and a default answer is displayed. The user can select the default answer by simply striking the "return" key, or he can enter a number. The number he enters is checked for proper syntax and is also checked to assure that it lies within known bounds. In this way, physically unreasonable data is rejected. The system is also capable of displaying "help" messages for inexperienced or forgetful users.

<u>Structure Diagrams</u>. The software was designed using structure diagrams. The elements of a structure diagram are shown in Figure 2. A simple structure diagram is shown in Figure 3. Structure diagrams are read from left to right within a vertical level. Each lower vertical level expands upon elements of the level above. In the case of the decision box, only one path to the lower level is taken, and so it is an exception to the left to right rule.

The use of structure diagrams has numerous advantages:

1) It is easy to see the overall picture.
2) They give as much detail as desired.
3) They are simple to learn and to use.
4) They provide a clear and concise common ground for discussions between software engineers and scientists.

We have also found structure diagrams to be excellent for software documentation purposes.

Structure diagrams for some of the system are shown in Figures 4 to 6. Figure 4 is the very first diagram which shows the general structure of the software for displaying a technique menu. Figure 5 shows the structure for selecting an instrumental technique and Figure 6 shows the choices available after the technique has been chosen. As can be seen from the boxes labeled "OTHERS", each section allows further software modules to be added when available. These diagrams also show the path the software can take back and forth between each technique or process.

Figures 7 and 8 are actual menus as they appear to the user as is Figure 9 to be discussed later.

Software. Software has been developed for acquiring, storing, recalling, and processing both ESCA/UPS and Auger spectra. The data is acquired from a Nicolet Model 1074 multichannel analyzer via a RS-232 serial link to the computer.

Once acquired the data is displayed as a spectrum. After viewing the data, the user may decide to save it or try again. If he decides to save it, the data is saved on the disk and the user must enter the pertinent labeling information.

This information is broken down into four categories:

1) Sample accounting.
2) Sample history.
3) Sputtering parameters.
4) Experimental parameters

Once this data is entered, the user can review it for accuracy before storing it. In order to make the labeling process easier, the user can instruct the system to provide as default answers the labels of any previously labeled spectrum. Often, this means that the user need only change a very few items.

The data processing techniques currently available are given in Figure 9, and the list is continuing to grow. All the data processing techniques make extensive use of interactive graphics and menus. Since the user is allowed to manipulate up to 20 spectra at one time, all the data processing techniques prompt the user with a menu of the names of the spectra available. Each spectrum is named by the user (separate from the spectrum's disk storage name) when it is recalled from the disk. This allows the user to give the spectrum a meaningful name.

Figure 10 shows a computer generated summary of a spectrum which has been processed in various ways. The names are chosen by the user and reflect what has been done to the original spectrum.

We are currently developing five additional data processing techniques. These are:

1) Multiple overlay plots
2) Normalize
3) Add/subtract spectra
4) Differentiate
5) Atomic abundance calculations

In the next few years, we hope to expand the system to include:

1) SIMS
2) Data Base Capabilities
3) Expanded Data Processing
4) Data Analysis Capabilities

Beyond the next few years, we look to:

1) Additional Surface Science Techniques, i.e. EELS and LEEDS
2) Artificial Intelligence Methods for Sample Analysis.

FIGURES

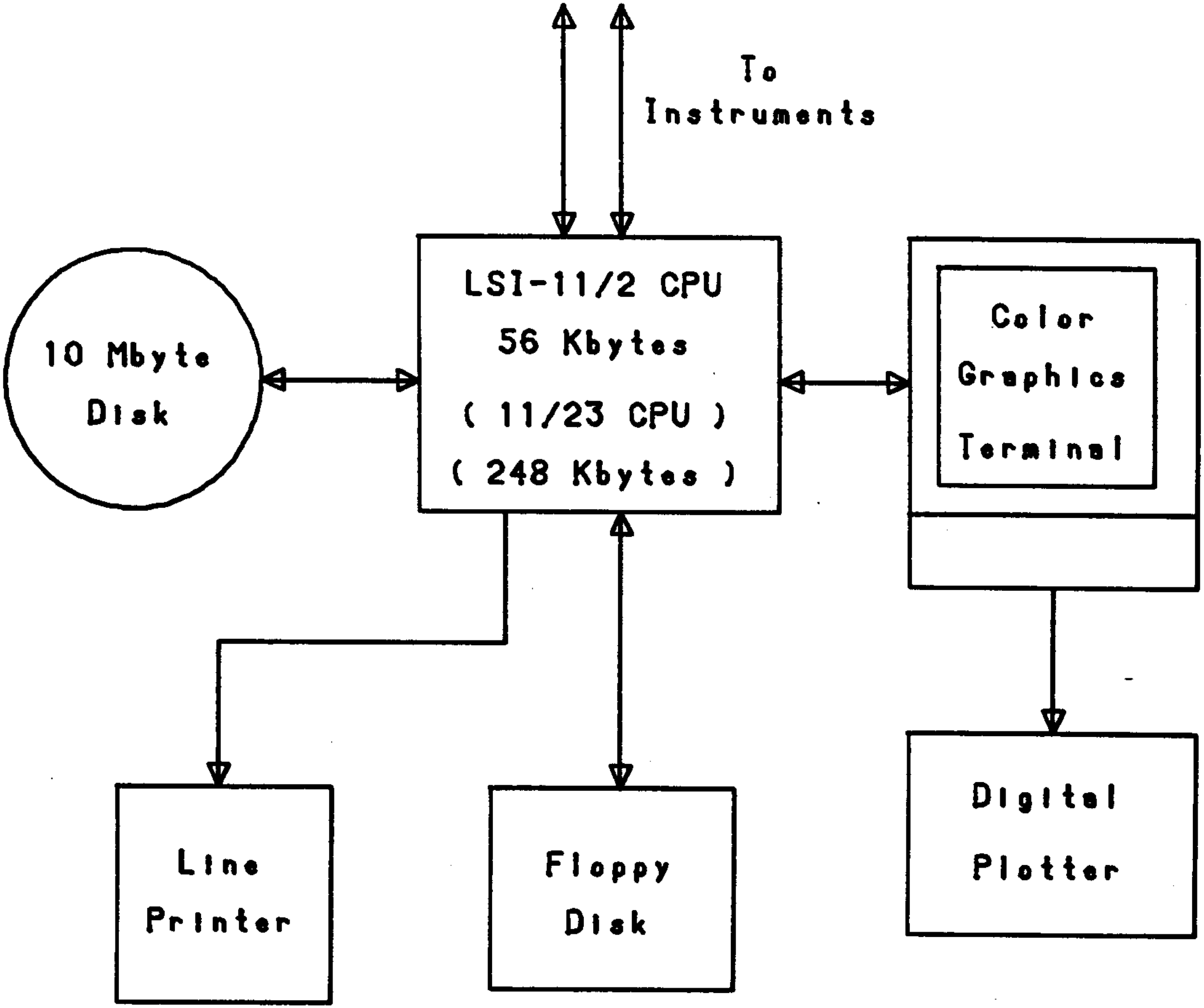

To
Instruments
LSI-11/2 CPU
56 Kbytes
(11/23 CPU)
(248 Kbytes)
10 Mbyte
Disk
Color
Graphics
Terminal
Line
Printer
Floppy
Disk
Digital
Plotter

FIGURE 1.

ELEMENTS OF STRUCTURE DIAGRAMS

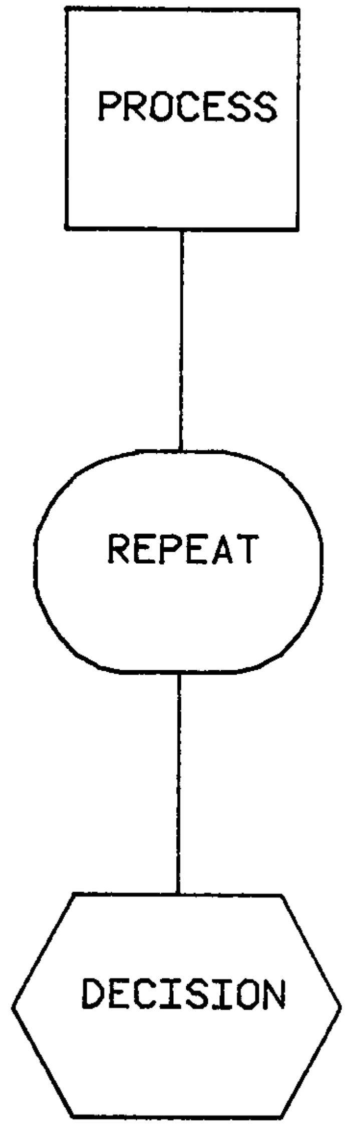


FIGURE 2.

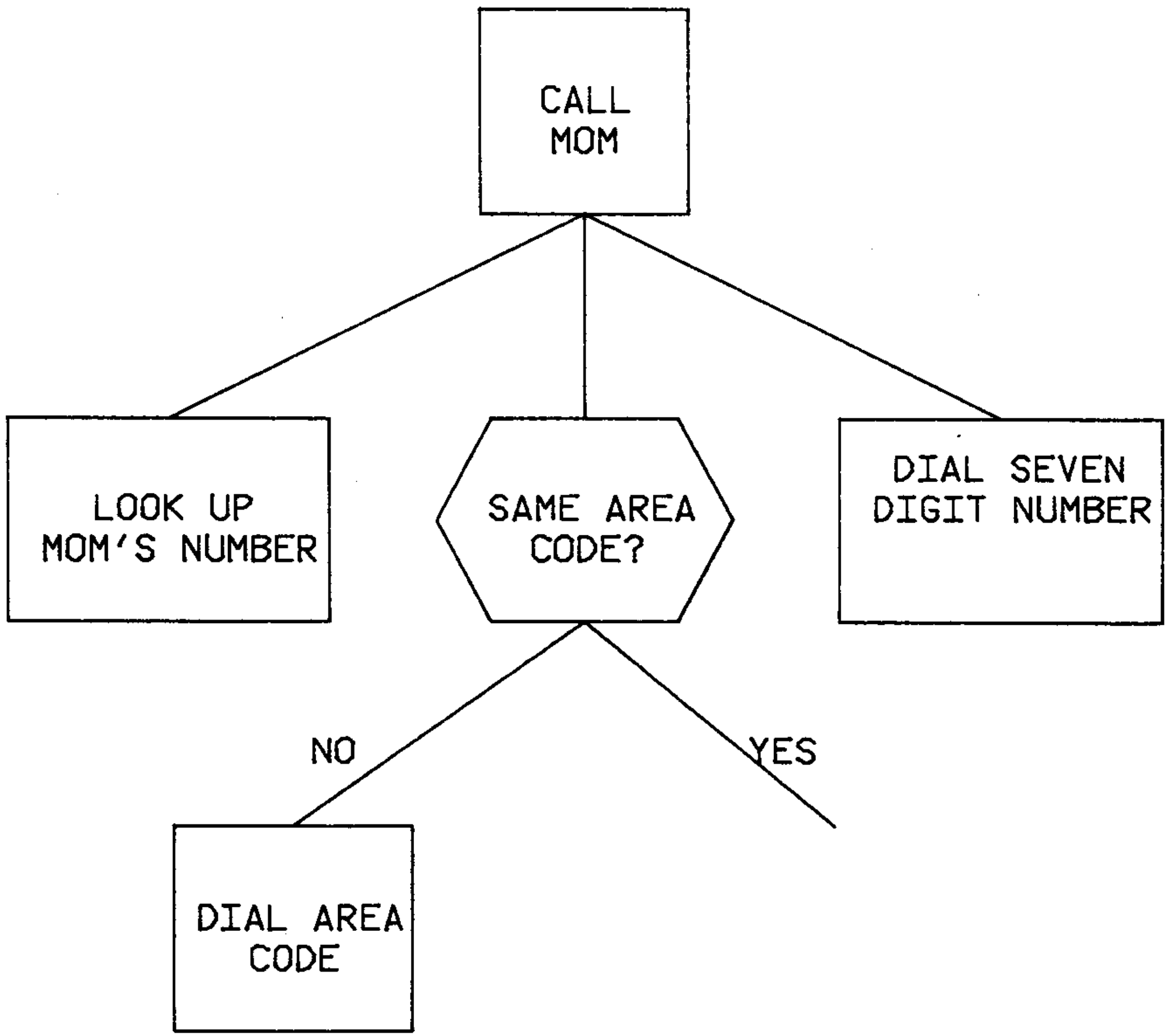

CALL
MOM
LOOK UP
MOM'S NUMBER
SAME AREA
CODE?
DIAL SEVEN
DIGIT NUMBER
NO
YES
DIAL AREA
CODE

FIGURE 3.

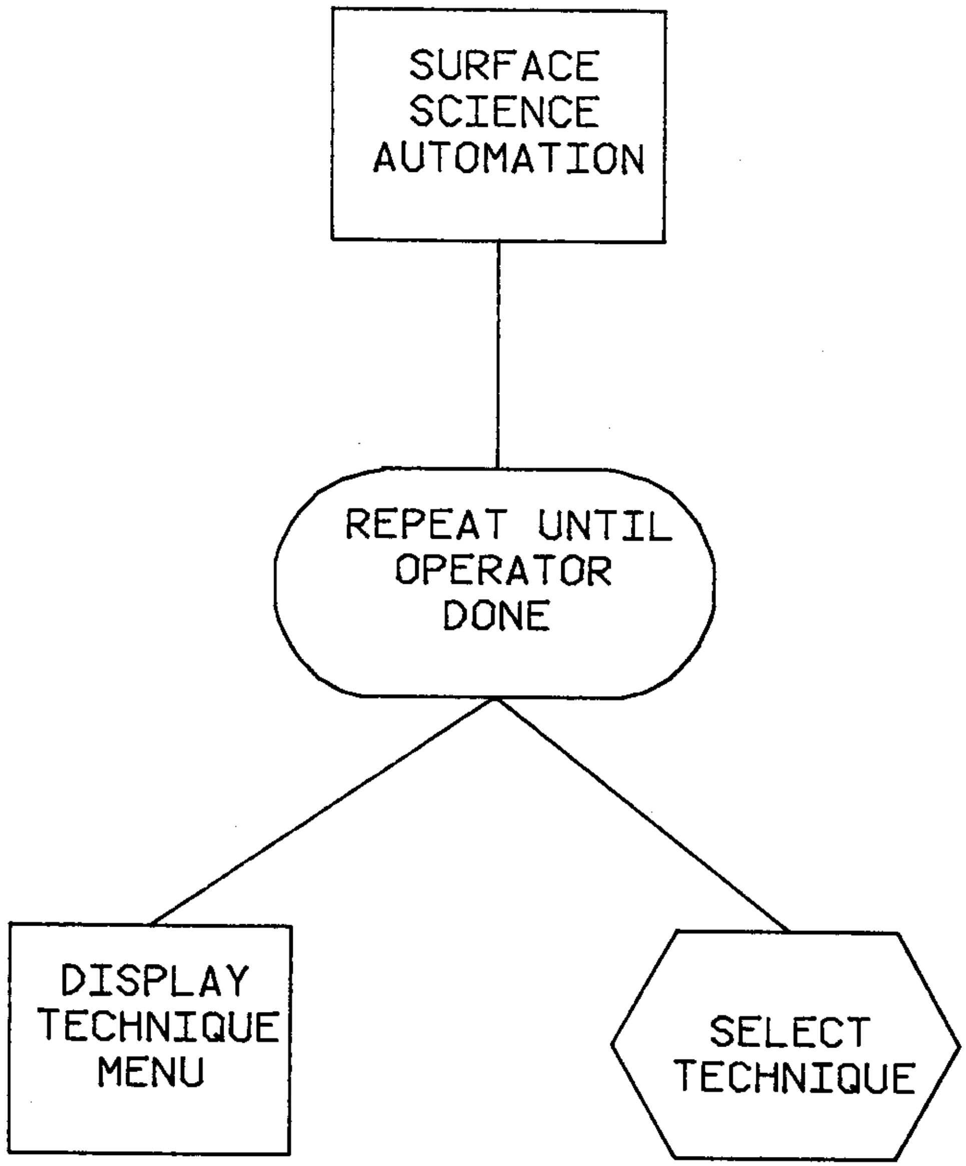

SURFACE
SCIENCE
AUTOMATION
REPEAT UNTIL
OPERATOR
DONE
DISPLAY
TECHNIQUE
MENU
SELECT
TECHNIQUE

FIGURE 4.

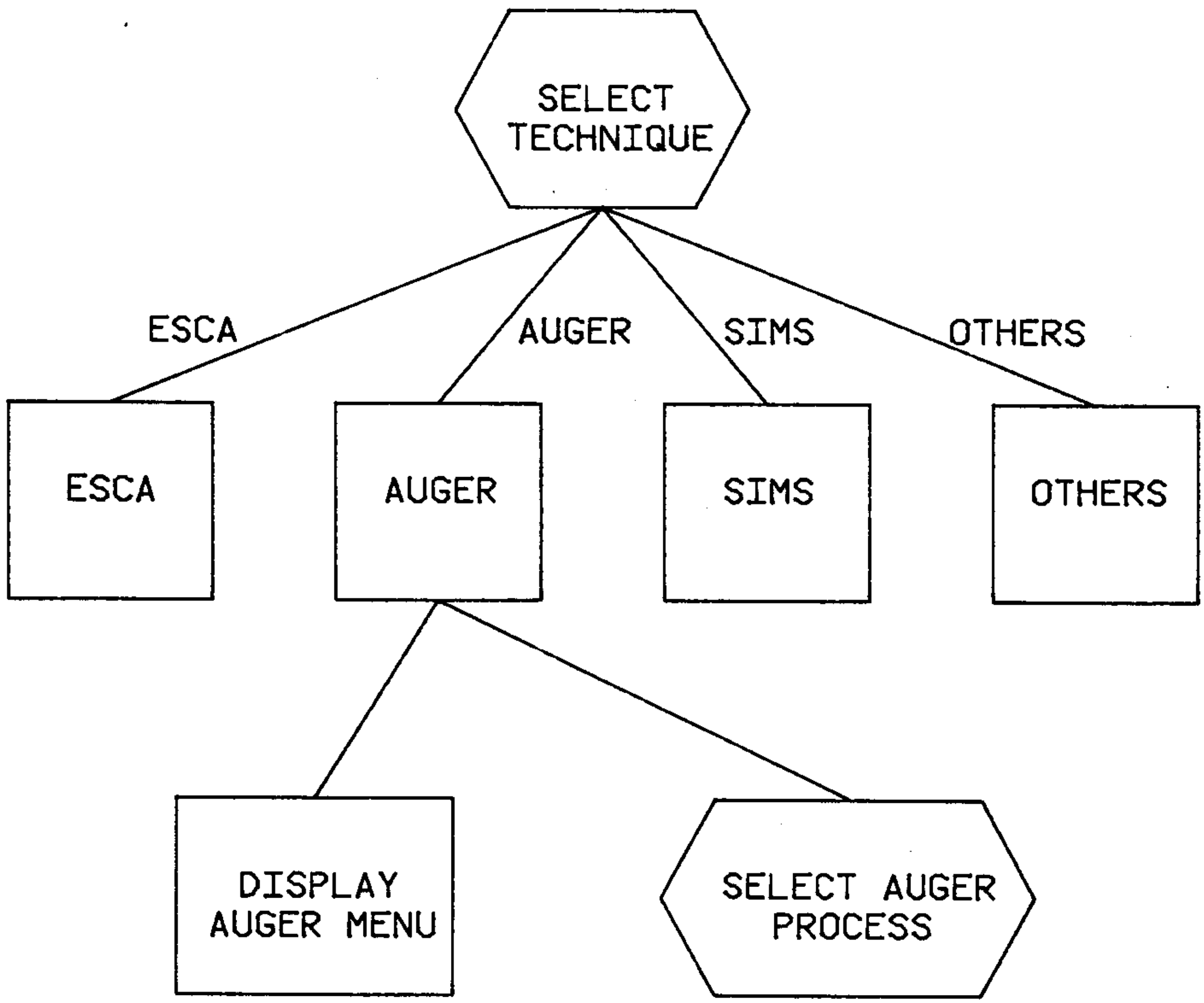
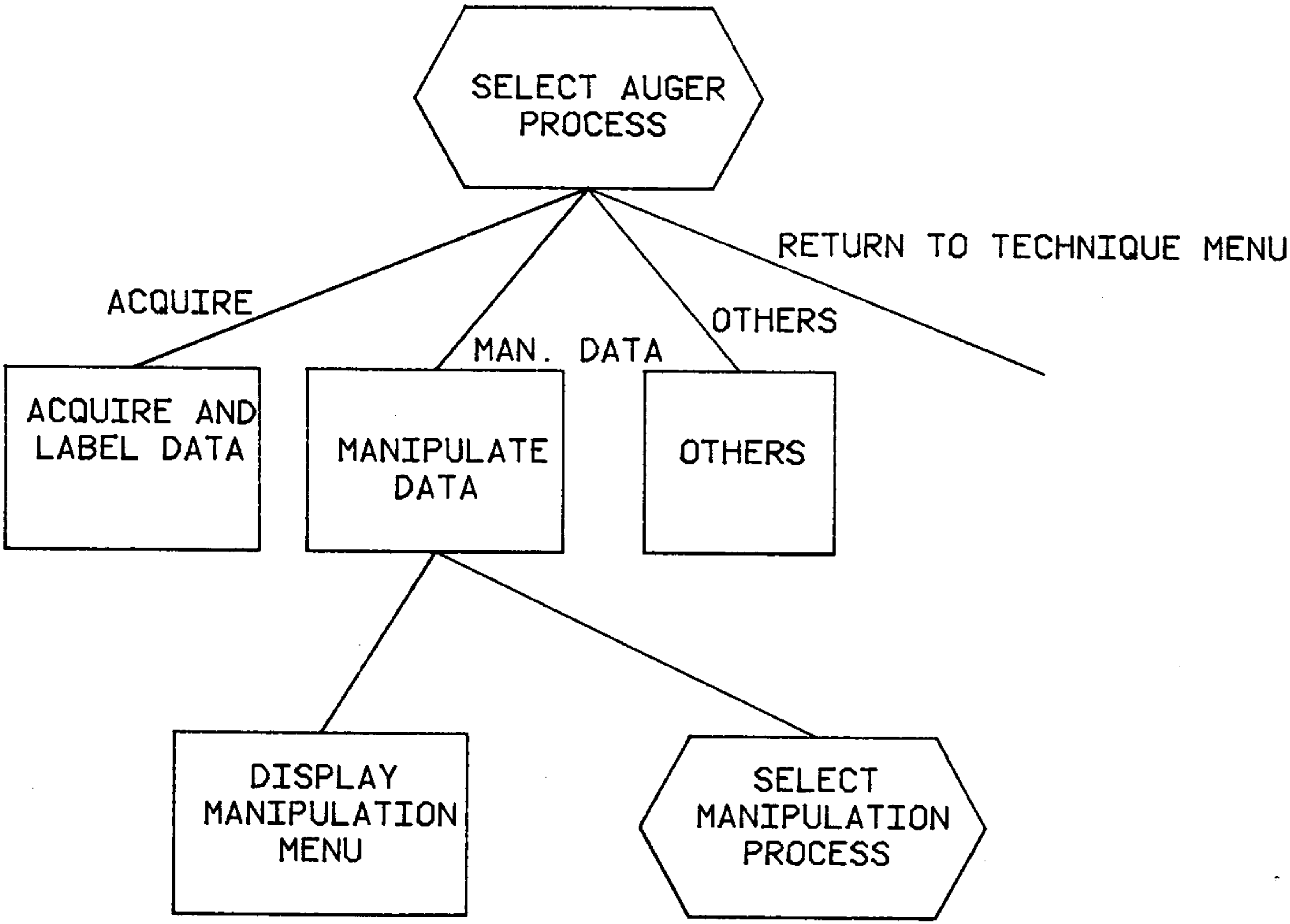

SELECT
TECHNIQUE
ESCA
AUGER
SIMS
OTHERS
ESCA
AUGER
SIMS
OTHERS
DISPLAY
AUGER MENU
SELECT AUGER
PROCESS

FIGURE 5.



SELECT AUGER PROCESS
ACQUIRE
MAN. DATA
OTHERS
RETURN TO TECHNIQUE MENU
ACQUIRE AND LABEL DATA
MANIPULATE DATA
OTHERS
DISPLAY MANIPULATION MENU
SELECT MANIPULATION PROCESS

FIGURE 6.

SELECT PROPER TECHNIQUE

1. ALL DONE. RETURN TO RT-11.

2. ESCA/UPS

3. AUGER

4. SIMS

FIGURE 7.

SELECT A PROGRAM TO PROCESS ESCA DATA

1. ALL DONE. RETURN TO TECHNIQUE MENU.

2. ACQUIRE/LABEL

3. INTERACT

FIGURE 8.

DATA MANIPULATION OPTIONS

1. EXIT DATA MANIPULATION
2. DEFINE A NEW SPECTRUM
3. LIST/RENAME SPECTRA AVAILABLE
4. DELETE A SPECTRUM
5. DISPLAY/PLOT A SPECTRUM
6. READ POINTS FROM A SPECTRUM
7. ZOOM A SPECTRUM
8. SMOOTH A SPECTRUM
9. CALC. PEAK AREAS
10. SUBTRACT BASELINE
11. INTEGRATE A SPECTRUM
12. RECALIBRATE ENERGY AXIS
13. REMOVE SPIKES

FIGURE 9.

#	NAME	ORIGIN	XMIN	XMAX	NPTS	YMIN	YMAX
1	SAMPLE	CUSGBQ	1000.	0.	1022	748.	44681.
2	ZOOM	CUSGBQ	453.	368.	88	8775.	28765.
3	ZOOMED	CUSGBQ	359.	179.	160	1594.	19161.
4	SPIKE REMOVED	CUSGBQ	1000.	0.	1022	748.	45043.
5	ZOOMED - BKGD	CUSGBQ	341.	185.	160	-428.	11824.
6	ZOOM WITHOUT SPIKE	CUSGBQ	453.	368.	88	8775.	14990.
7	LOW ENERGY ZOOM	CUSGBQ	198.	0.	203	748.	2033.
8	SMOOTHED LOW ENERGY	CUSGBQ	198.	0.	203	792.	1984.

FIGURE 10.